



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:45 PM GMT

PDB ID : 3CX3
Title : Crystal structure Analysis of the Streptococcus pneumoniae AdcAII protein
Authors : Loisel, E.; Durmort, C.; Jacquamet, L.
Deposited on : 2008-04-23
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

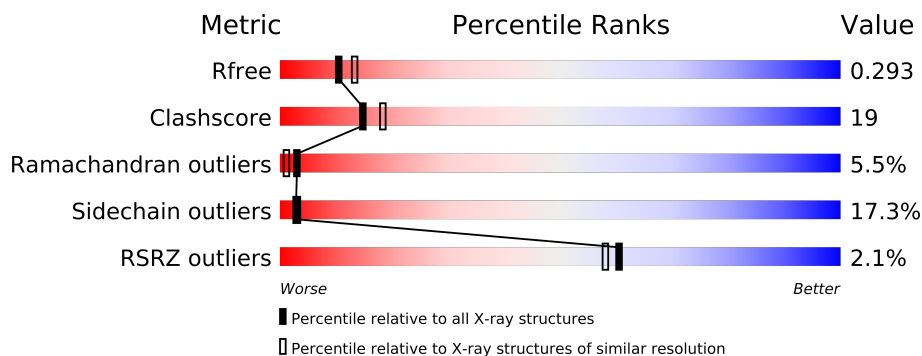
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	284	
1	B	284	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NA	A	312	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4280 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	Se	0	3	0
			2087	1327	341	414	5			
1	B	260	Total	C	N	O	Se	0	1	0
			2045	1301	333	406	5			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Na	0	0
			2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

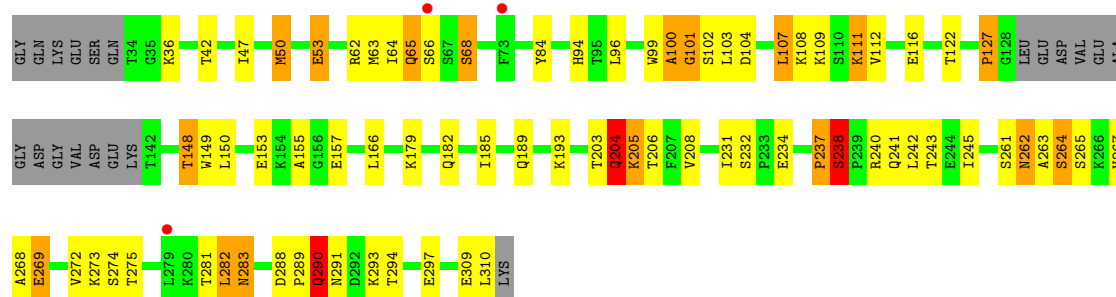
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total	O	0	0
			72	72		
4	B	72	Total	O	0	0
			72	72		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

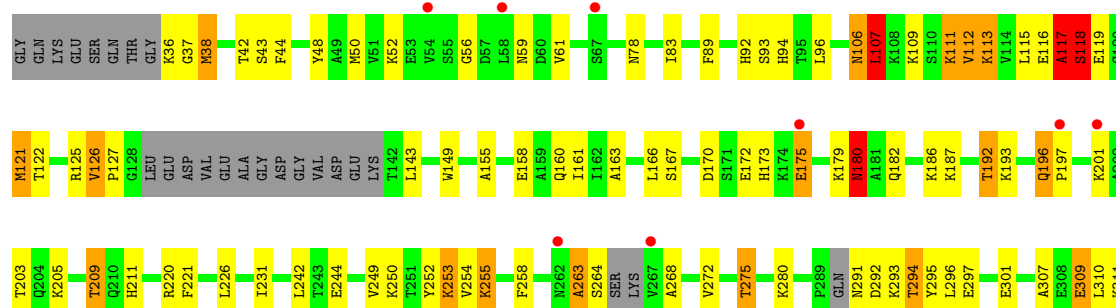
• Molecule 1: Lipoprotein

Chain A: 



• Molecule 1: Lipoprotein

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.76Å 63.26Å 151.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.90 – 2.40 44.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.90-2.40) 97.9 (44.92-2.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.295 0.224 , 0.293	Depositor DCC
R_{free} test set	1064 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 21264 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4280	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/2127	0.80	4/2865 (0.1%)
1	B	0.55	0/2081	0.77	2/2799 (0.1%)
All	All	0.57	0/4208	0.79	6/5664 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	1	4
All	All	1	8

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	SER	N-CA-C	9.78	137.40	111.00
1	A	282	LEU	CA-CB-CG	6.57	130.41	115.30
1	A	101	GLY	N-CA-C	-5.83	98.53	113.10
1	B	117	ALA	N-CA-C	5.39	125.57	111.00
1	A	205	LYS	N-CA-C	5.36	125.46	111.00
1	A	238	SER	C-N-CD	-5.21	109.13	120.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	118	SER	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	PRO	Peptide
1	A	204	GLN	Peptide
1	A	264	SER	Peptide
1	A	289	PRO	Peptide
1	B	107	LEU	Peptide
1	B	117	ALA	Peptide
1	B	118	SER	Peptide
1	B	175	GLU	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2087	0	23	35	0
1	B	2045	0	16	45	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	72	0	0	7	0
4	B	72	0	0	5	0
All	All	4280	0	39	80	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (80) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:192:THR:C	1:B:196:GLN:NE2	1.94	1.21
1:B:192:THR:O	1:B:196:GLN:NE2	1.82	1.13
1:B:121:MSE:CE	1:B:161:ILE:CD1	2.48	0.92
1:A:50:MSE:CE	1:A:155:ALA:O	2.23	0.85
1:A:63:MSE:O	1:A:65:GLN:CG	2.25	0.84
1:A:309:GLU:O	1:A:310:LEU:HG	1.82	0.79
1:A:203:THR:O	1:A:310:LEU:HD22	1.80	0.79
1:B:291:ASN:CB	1:B:292:ASP:CA	2.65	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:92:HIS:O	1:B:118:SER:CB	2.36	0.73
1:B:117:ALA:O	1:B:161:ILE:CG2	2.37	0.72
1:A:53:GLU:OE1	4:A:382:HOH:O	2.08	0.72
1:A:99:TRP:O	1:A:100:ALA:CB	2.37	0.71
1:B:52:LYS:O	1:B:56:GLY:N	2.32	0.63
1:A:310:LEU:HD11	4:A:368:HOH:O	1.98	0.62
1:B:307:ALA:C	1:B:309:GLU:N	2.54	0.59
1:B:193:LYS:N	1:B:196:GLN:NE2	2.50	0.59
1:B:173:HIS:CE1	4:B:335:HOH:O	2.55	0.58
1:B:310:LEU:HB2	4:B:357:HOH:O	2.04	0.57
1:B:38:MSE:O	1:B:59:ASN:ND2	2.37	0.57
1:A:64:ILE:O	1:A:66:SER:N	2.37	0.57
1:A:204:GLN:NE2	4:A:371:HOH:O	2.37	0.56
1:B:50:MSE:CE	1:B:155:ALA:O	2.53	0.56
1:B:252:TYR:O	1:B:253:LYS:CB	2.54	0.55
1:B:264:SER:O	1:B:268:ALA:N	2.40	0.55
1:B:126:VAL:CG2	1:B:231:ILE:CD1	2.85	0.55
1:A:290:GLN:O	1:A:291:ASN:OD1	2.25	0.54
1:B:83:ILE:O	1:B:112:VAL:CG1	2.56	0.54
1:A:148:THR:O	1:A:150:LEU:N	2.40	0.54
1:A:263:ALA:O	1:A:265:SER:N	2.40	0.54
1:A:288:ASP:OD2	1:A:290:GLN:NE2	2.42	0.53
1:B:196:GLN:CG	1:B:221:PHE:CE1	2.91	0.53
1:B:163:ALA:O	1:B:166:LEU:O	2.27	0.53
1:A:101:GLY:O	1:A:102:SER:CB	2.54	0.53
1:B:293:LYS:O	1:B:294:THR:O	2.27	0.52
1:B:126:VAL:CB	1:B:127:PRO:CD	2.87	0.52
1:B:37:GLY:O	1:B:38:MSE:CB	2.57	0.52
1:A:94:HIS:ND1	1:A:116:GLU:OE1	2.43	0.52
1:B:179:LYS:O	1:B:180:ASN:CB	2.58	0.51
1:A:290:GLN:O	1:A:291:ASN:CG	2.51	0.49
1:B:92:HIS:ND1	1:B:158:GLU:OE2	2.46	0.49
1:A:274:SER:OG	1:A:275:THR:N	2.45	0.49
1:A:84:TYR:OH	1:A:104:ASP:N	2.46	0.48
1:A:237:PRO:O	1:A:241:GLN:NE2	2.46	0.48
1:A:268:ALA:O	1:A:269:GLU:C	2.52	0.47
1:B:170:ASP:OD2	1:B:173:HIS:CD2	2.67	0.47
1:B:249:VAL:CG1	1:B:275:THR:CG2	2.92	0.47
1:B:258:PHE:CE1	1:B:310:LEU:CG	2.97	0.46
1:B:126:VAL:O	1:B:127:PRO:C	2.51	0.46
1:B:192:THR:CB	1:B:196:GLN:NE2	2.78	0.46
1:B:111:LYS:NZ	4:B:351:HOH:O	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:238:SER:OG	1:A:241:GLN:N	2.48	0.46
1:B:112:VAL:O	1:B:113:LYS:C	2.54	0.46
1:B:307:ALA:O	1:B:309:GLU:N	2.49	0.46
1:B:272:VAL:O	1:B:275:THR:O	2.34	0.46
1:B:310:LEU:O	1:B:311:LYS:HG3	2.17	0.45
1:B:94:HIS:ND1	1:B:116:GLU:OE2	2.49	0.45
1:B:149:TRP:O	1:B:295:TYR:OH	2.34	0.45
1:A:153:GLU:CG	4:A:367:HOH:O	2.64	0.45
1:A:64:ILE:O	1:A:65:GLN:C	2.55	0.45
1:B:209:THR:CG2	1:B:211:HIS:O	2.65	0.45
1:A:261:SER:O	1:A:262:ASN:C	2.56	0.44
1:A:309:GLU:O	1:A:310:LEU:CG	2.57	0.44
1:A:109:LYS:O	1:A:109:LYS:CG	2.66	0.43
1:B:48:TYR:CZ	1:B:52:LYS:NZ	2.86	0.43
1:A:297:GLU:CG	4:A:333:HOH:O	2.66	0.43
1:B:166:LEU:O	1:B:167:SER:OG	2.35	0.43
1:A:99:TRP:O	1:A:99:TRP:CG	2.68	0.43
1:B:113:LYS:NZ	4:B:351:HOH:O	2.52	0.43
1:A:94:HIS:N	1:A:116:GLU:OE1	2.53	0.42
1:A:203:THR:O	1:A:310:LEU:CD2	2.60	0.42
1:B:255:LYS:CG	1:B:311:LYS:HG2	2.50	0.42
1:A:238:SER:OG	1:A:240:ARG:N	2.53	0.42
1:A:68:SER:CA	4:A:339:HOH:O	2.66	0.41
1:A:111:LYS:N	1:A:111:LYS:CD	2.83	0.41
1:A:283:ASN:ND2	4:A:365:HOH:O	2.53	0.41
1:B:196:GLN:N	1:B:197:PRO:CD	2.84	0.41
1:B:263:ALA:O	1:B:264:SER:C	2.59	0.40
1:A:272:VAL:O	1:A:274:SER:N	2.55	0.40
1:B:172:GLU:CG	4:B:335:HOH:O	2.69	0.40
1:B:89:PHE:O	1:B:115:LEU:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	263/284 (93%)	212 (81%)	34 (13%)	17 (6%)	2	1
1	B	253/284 (89%)	212 (84%)	29 (12%)	12 (5%)	4	2
All	All	516/568 (91%)	424 (82%)	63 (12%)	29 (6%)	3	1

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	SER
1	A	107	LEU
1	A	205	LYS
1	A	237	PRO
1	A	262	ASN
1	A	264	SER
1	A	290	GLN
1	B	38	MSE
1	B	126	VAL
1	B	180	ASN
1	B	253	LYS
1	B	254	VAL
1	B	294	THR
1	A	36[A]	LYS
1	A	36[B]	LYS
1	A	65	GLN
1	A	100	ALA
1	A	293	LYS
1	B	107	LEU
1	B	113	LYS
1	B	118	SER
1	B	263	ALA
1	A	149	TRP
1	A	204	GLN
1	A	238	SER
1	A	273	LYS
1	B	119	GLU
1	B	106	ASN
1	A	127	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain

conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	230/242 (95%)	193 (84%)	37 (16%)	3	4
1	B	225/242 (93%)	183 (81%)	42 (19%)	2	2
All	All	455/484 (94%)	376 (83%)	79 (17%)	3	3

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	THR
1	A	47	ILE
1	A	50	MSE
1	A	53	GLU
1	A	62	ARG
1	A	96	LEU
1	A	103[A]	LEU
1	A	103[B]	LEU
1	A	107	LEU
1	A	108	LYS
1	A	111	LYS
1	A	112	VAL
1	A	122	THR
1	A	148	THR
1	A	157	GLU
1	A	166	LEU
1	A	179	LYS
1	A	182	GLN
1	A	185	ILE
1	A	189	GLN
1	A	193	LYS
1	A	204	GLN
1	A	206	THR
1	A	208	VAL
1	A	231	ILE
1	A	232	SER
1	A	234	GLU
1	A	242	LEU
1	A	243	THR
1	A	245	ILE
1	A	267	VAL
1	A	269	GLU
1	A	281	THR
1	A	282	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	283	ASN
1	A	290	GLN
1	A	294	THR
1	B	36	LYS
1	B	42	THR
1	B	43	SER
1	B	44	PHE
1	B	61	VAL
1	B	78	ASN
1	B	93	SER
1	B	96	LEU
1	B	106	ASN
1	B	107	LEU
1	B	109	LYS
1	B	111	LYS
1	B	112	VAL
1	B	118	SER
1	B	121	MSE
1	B	122	THR
1	B	125	ARG
1	B	143	LEU
1	B	160	GLN
1	B	175	GLU
1	B	180	ASN
1	B	182	GLN
1	B	186	LYS
1	B	187	LYS
1	B	192	THR
1	B	196	GLN
1	B	201	LYS
1	B	203	THR
1	B	205	LYS
1	B	209	THR
1	B	220	ARG
1	B	226	LEU
1	B	242	LEU
1	B	244	GLU
1	B	250	LYS
1	B	255	LYS
1	B	275	THR
1	B	280	LYS
1	B	296	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	297	GLU
1	B	301	GLU
1	B	309	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	264/284 (92%)	-0.01	3 (1%) 77 77	26, 55, 76, 90	0
1	B	260/284 (91%)	0.13	8 (3%) 47 44	24, 58, 83, 89	0
All	All	524/568 (92%)	0.06	11 (2%) 60 58	24, 56, 82, 90	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	VAL	4.9
1	A	66	SER	4.5
1	B	262	ASN	4.3
1	A	279	LEU	4.2
1	B	175	GLU	3.1
1	B	197	PRO	2.7
1	B	58	LEU	2.5
1	B	67	SER	2.4
1	B	201	LYS	2.4
1	B	54	VAL	2.1
1	A	73	PHE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NA	A	312	1/1	0.23	4.75	50,50,50,50	0
2	NA	A	313	1/1	0.17	0.76	54,54,54,54	0
3	ZN	B	312	1/1	0.13	-0.28	37,37,37,37	0
3	ZN	A	314	1/1	0.11	-0.66	36,36,36,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.